Large-Scale First-Principles Molecular Dynamics Simulations on the BlueGene/L Platform using the Qbox Code

2005 Gordon Bell Award - Finalist

François Gygi, Erik W. Draeger, Bronis de Supinski, and Robert K. Yates (CASC),
Franz Franchetti (Carnegie Mellon University), Stefan Kral, Jeurgen Lorenz and Christoph Ueberhueber (Vienna University of Technology), John A. Gunnels and James C. Sexton (IBM)

First-Principles Molecular Dynamics (FPMD) is an accurate, atomistic simulation approach that is routinely applied to a variety of areas including solid-state physics, chemistry, biochemistry and nanotechnology. FPMD enables one to perform predictive materials simulations, as no empirical or adjustable parameters are used to describe a given system. Instead, a quantum mechanical description of electrons is obtained by solving the Kohn–Sham equations within a pseudopotential plane-wave formalism. This rigorous first-principles treatment of electronic structure is computationally expensive and limits the size of tractable systems to a few hundred atoms on most currently available parallel computers. Developed specifically for large parallel systems at LLNL's Center for Applied Scientific Computing, the Qbox implementation of the FPMD method shows unprecedented performance and scaling on BlueGene/L.

Team members (L-R) Kim Yates (CASC), Christoph Ueberhueber (Vienna University of Technology), Franz Franchetti (Carnegie Mellon University), Erik Draeger, Francois Gygi, and Bronis de Supinski (CASC), as well as Bill Gropp (ANL).

Predicting the properties of metals under extreme conditions of temperature and pressure has been a longstanding goal of materials science and high-energy density physics. Under extreme conditions, some important properties of metals require simulations with a significantly larger number of atoms than have previously been feasible, for example the calculation of melting temperatures using the two-phase simulation technique and the calculation of defect energies and defect migration processes. Qbox simulations of 1000 molybdenum atoms (12,000 electrons) showed that a strong scaling parallel efficiency of 86% can be obtained between 1024 and 32,768 processors. Using 65,536 processors, we observed a sustained performance of up to 64 TFlops. This system is considerably larger than any previously feasible FPMD simulation and represents the next generation of predictive materials simulations.

UCRL-TR-217981